Introduction to Machine Learning

Finding the Nearest Neighborhood

Andres Mendez-Vazquez

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Outline

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Geometric Data Structures

We want to have data structures for

Organization of points, lines, planes, ... to support faster processing

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- Graphics – computing object intersections
- Data compression
  - Points are representatives of 2x2 blocks in an image
  - Nearest neighbor search

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KD Tree

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KD tree are guaranteed $\log_2 n$ depth where n is the number of points in the set.

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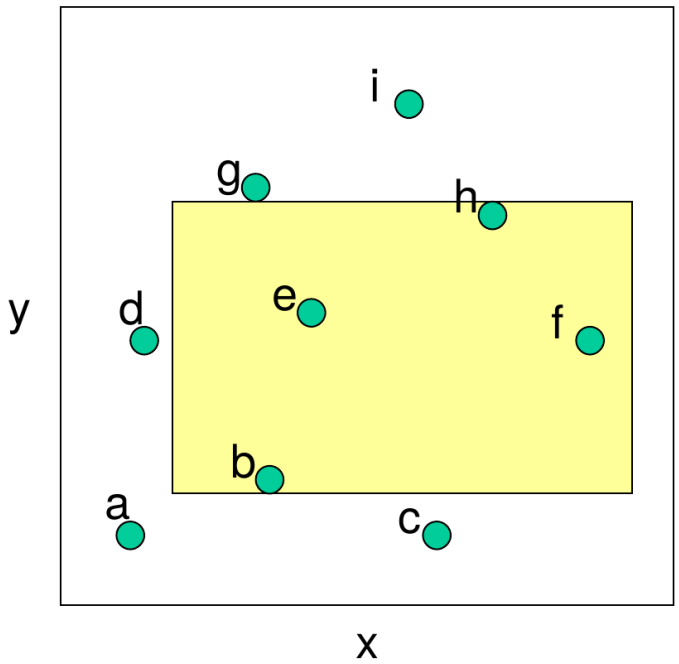
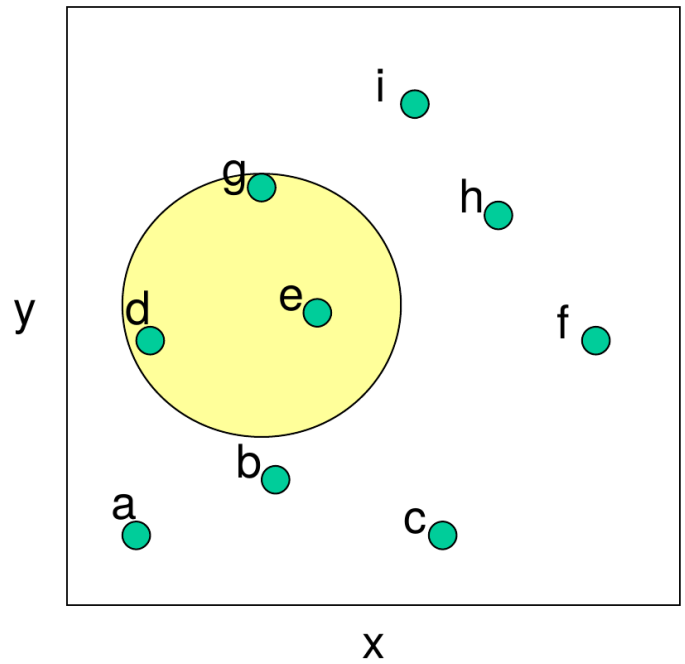
Example - Range Query

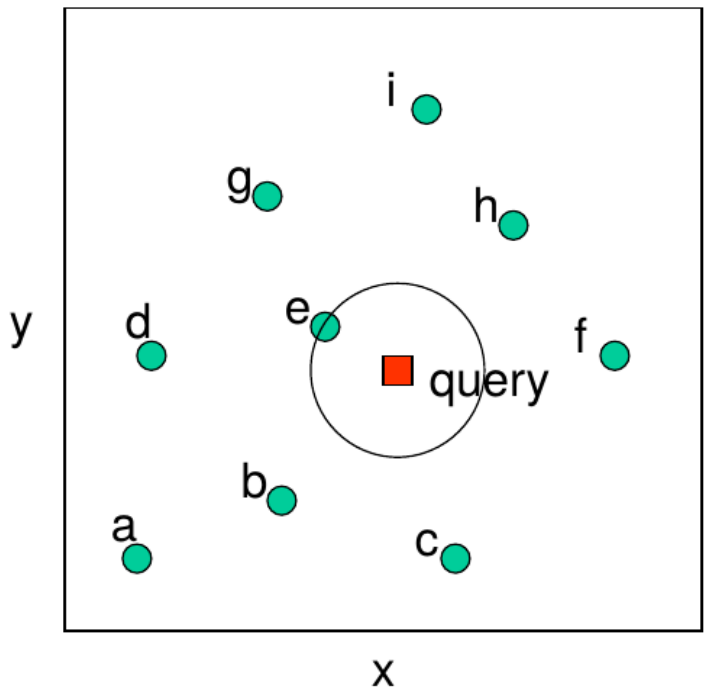


Rectangular query



Circular query

Nearest Neighbor Search



Nearest neighbor is e.

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We have the following procedure

Steps

1. If there is just one point, form a leaf with that point.
2. Otherwise, divide the points in half by a line perpendicular to one of the axes.
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Criterion I

Divide points perpendicular to the axis with widest spread.

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Divide in a round-robin fashion (book does it this way).

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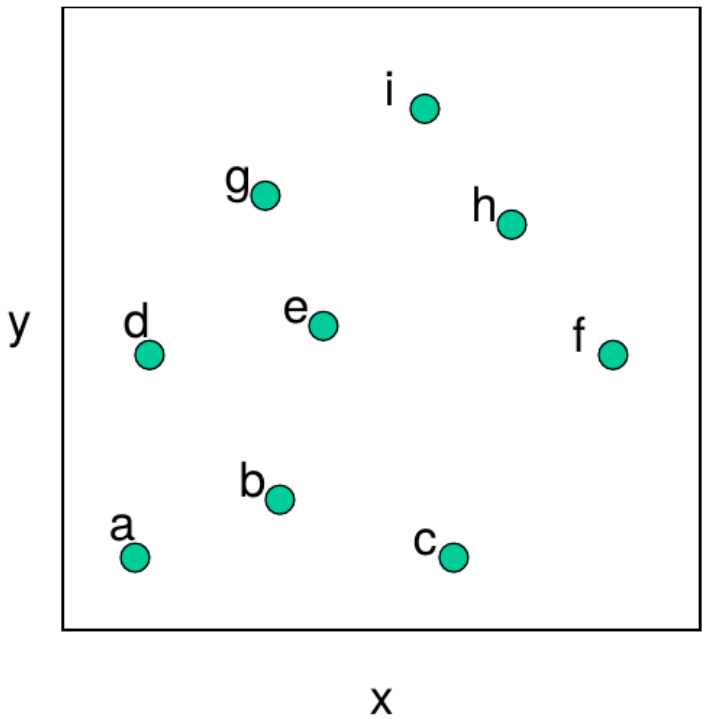

divide perpendicular to the widest spread.

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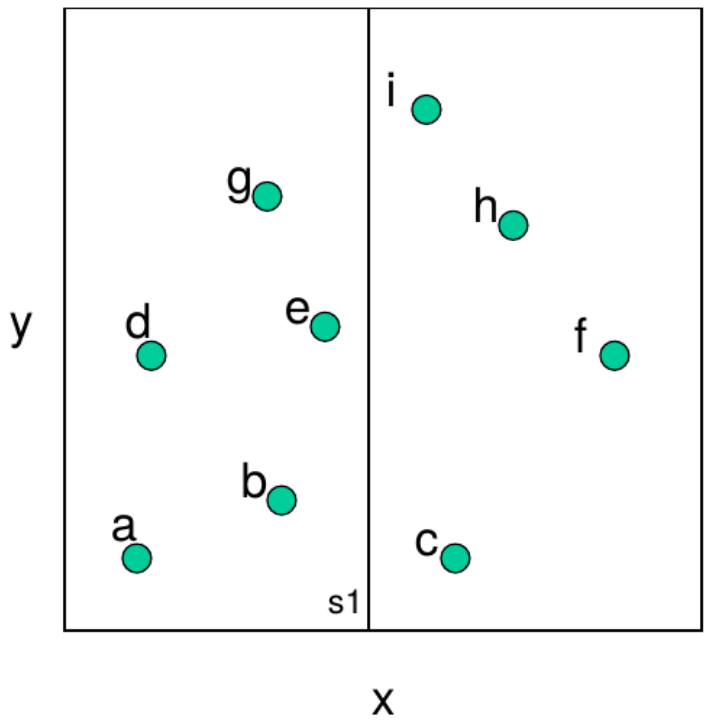

x
s1

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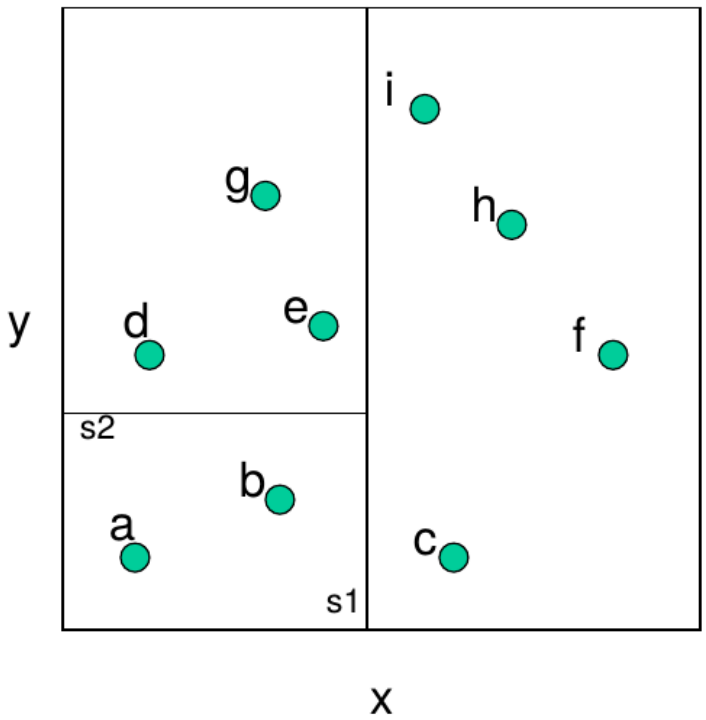

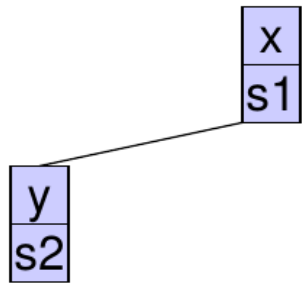

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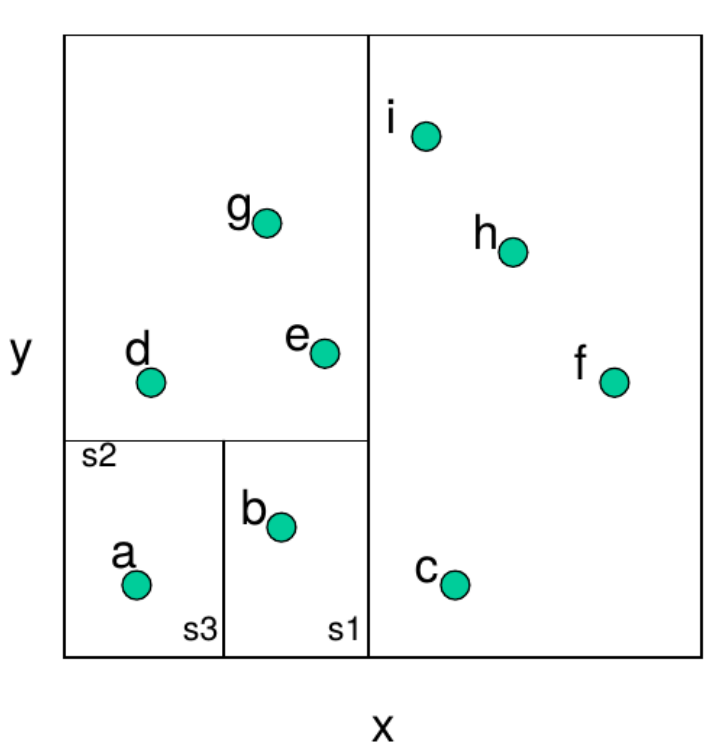

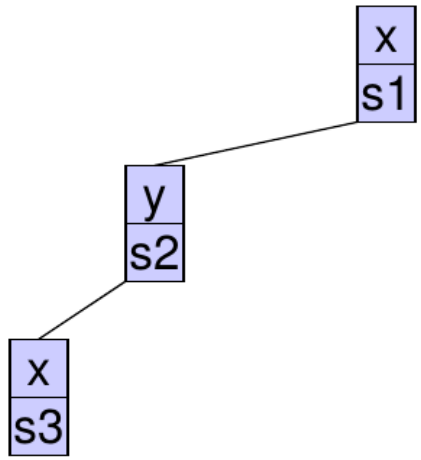

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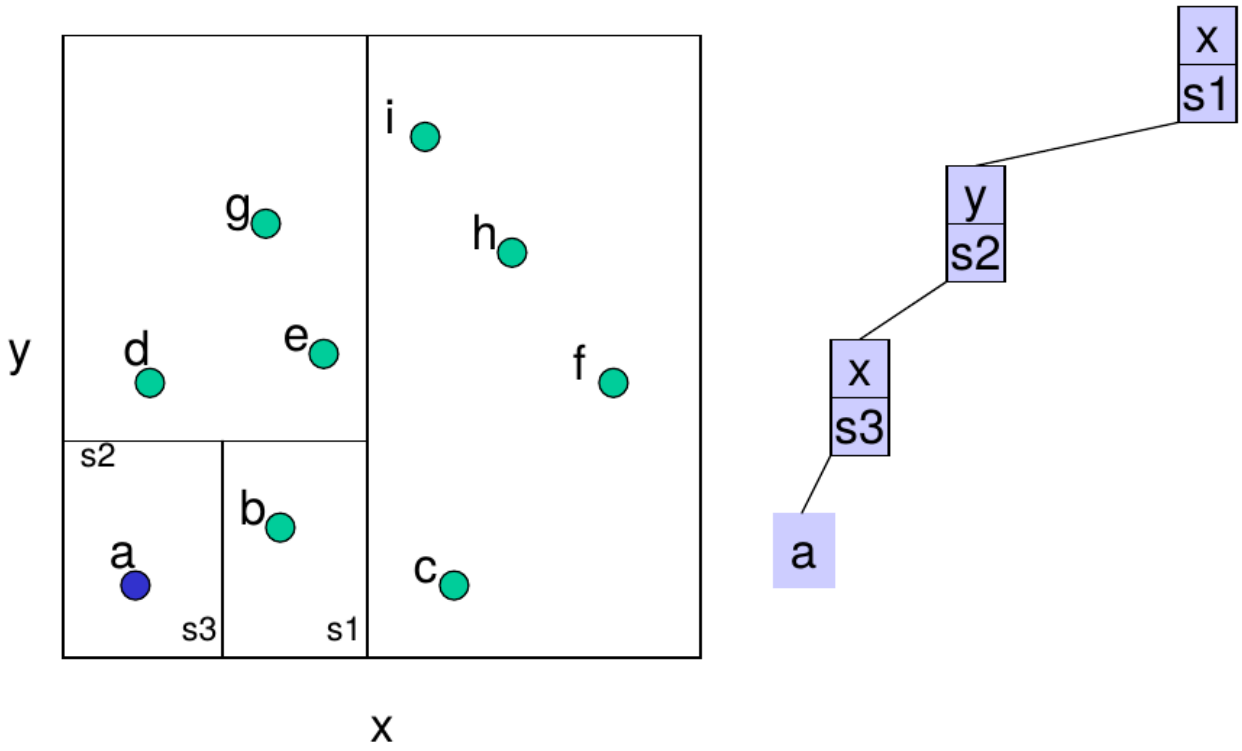

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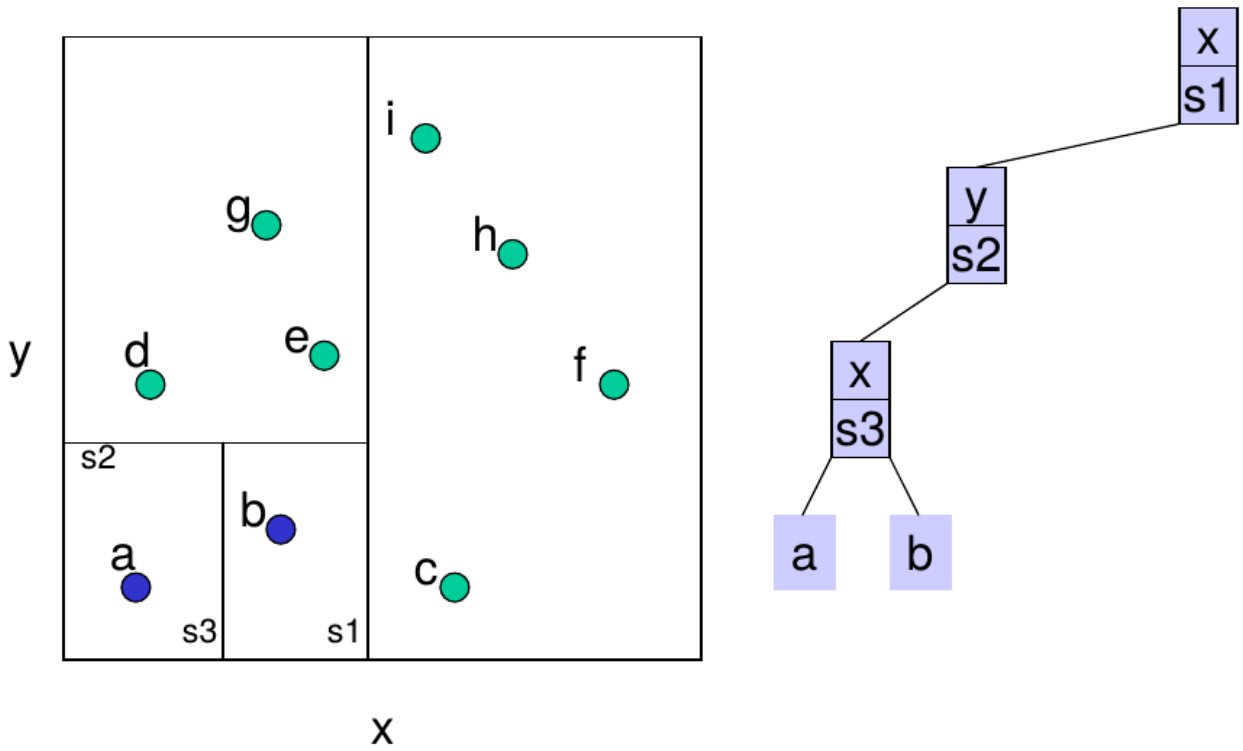

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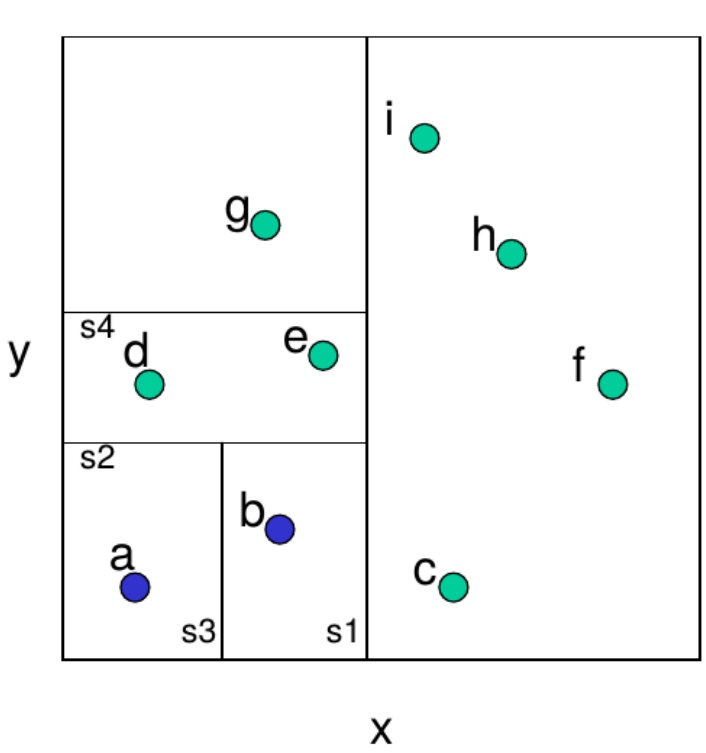

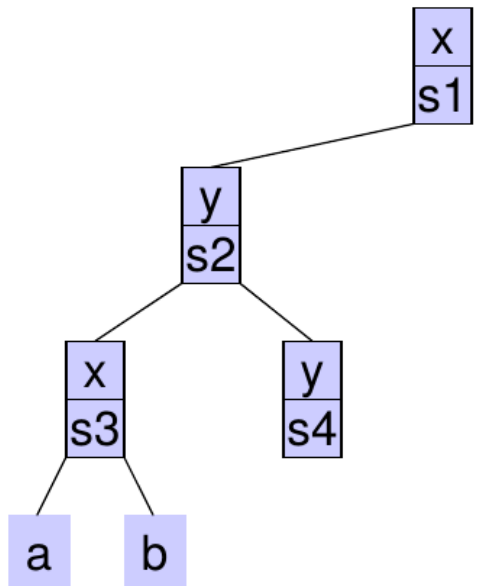

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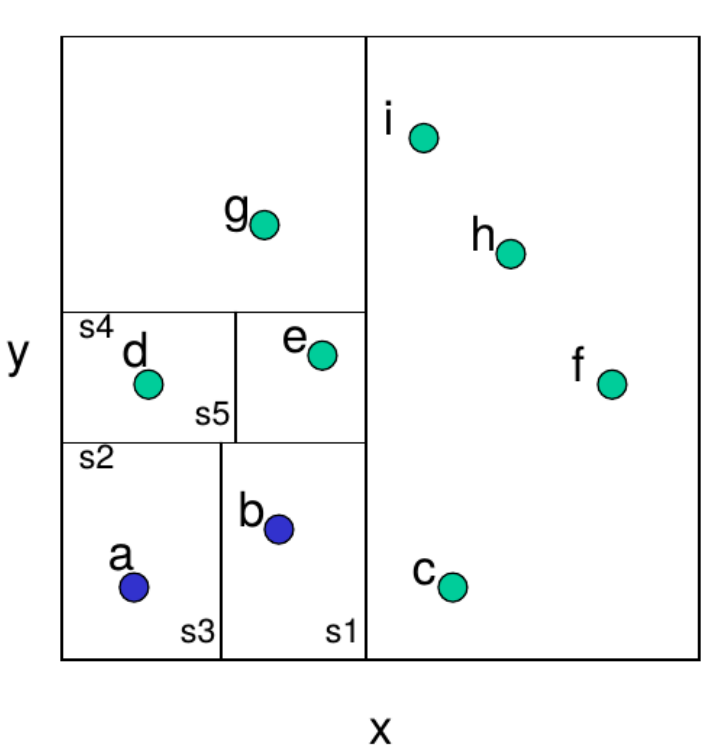

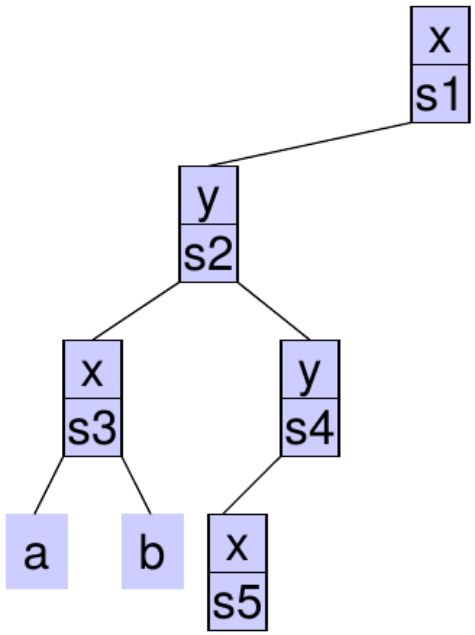

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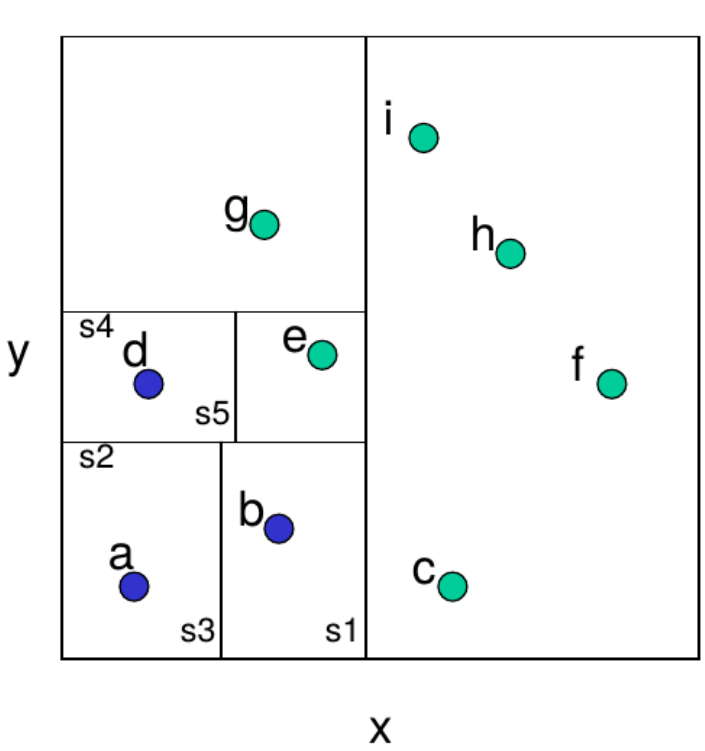

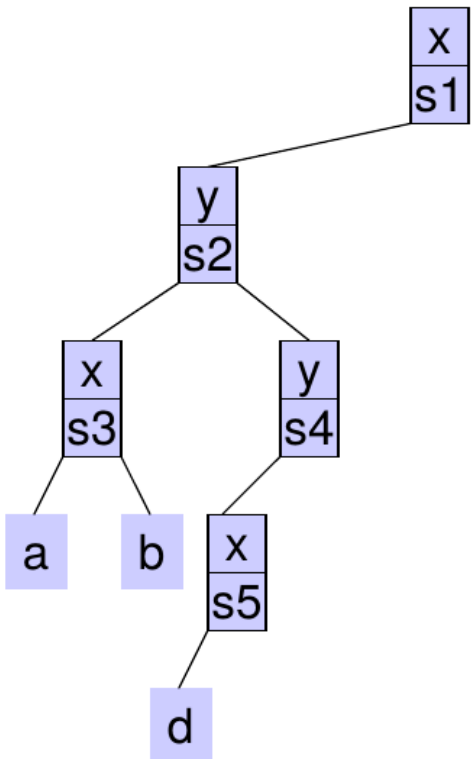

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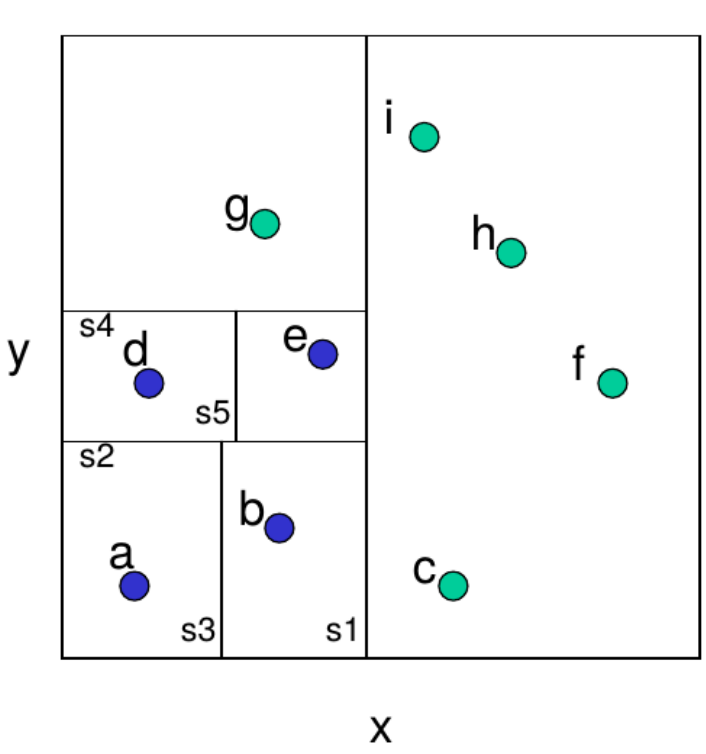

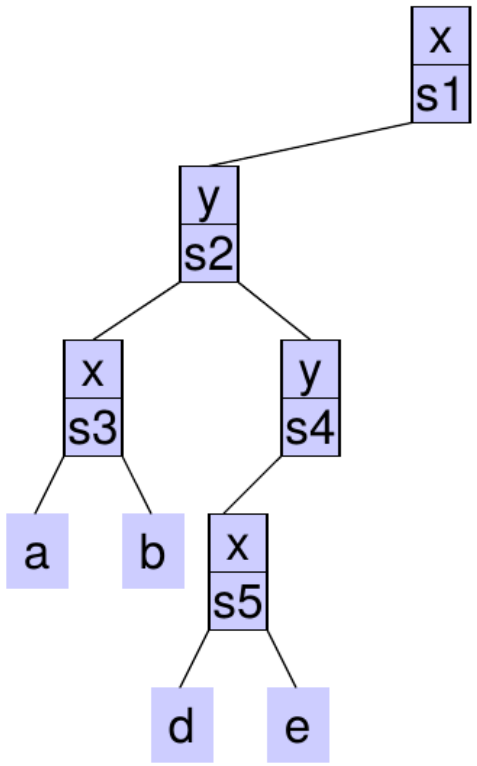

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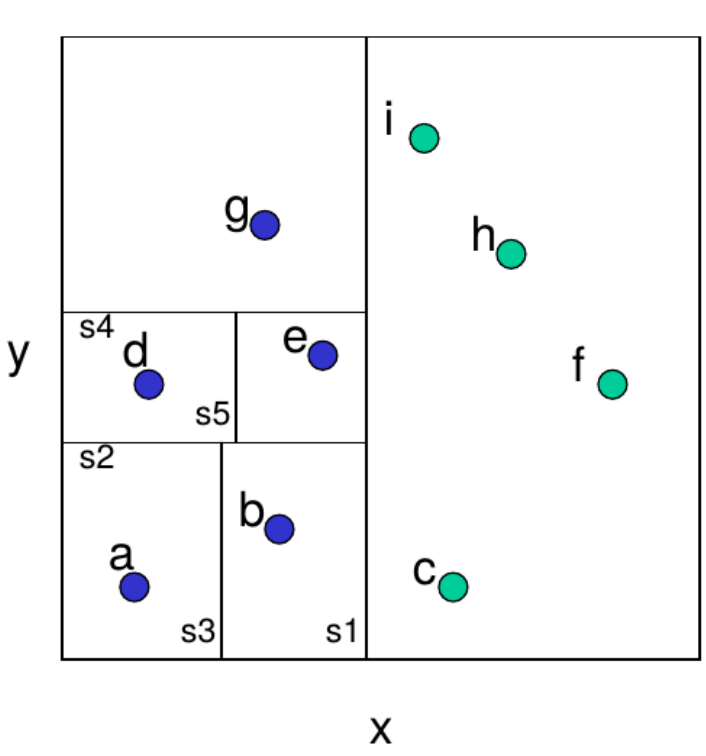
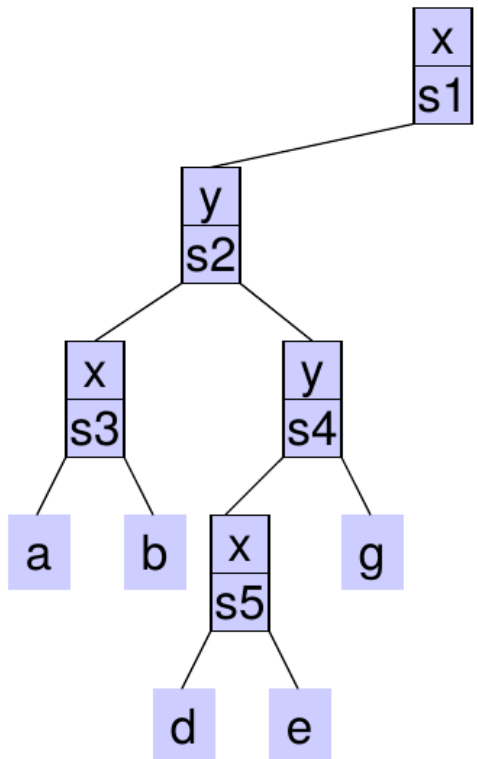
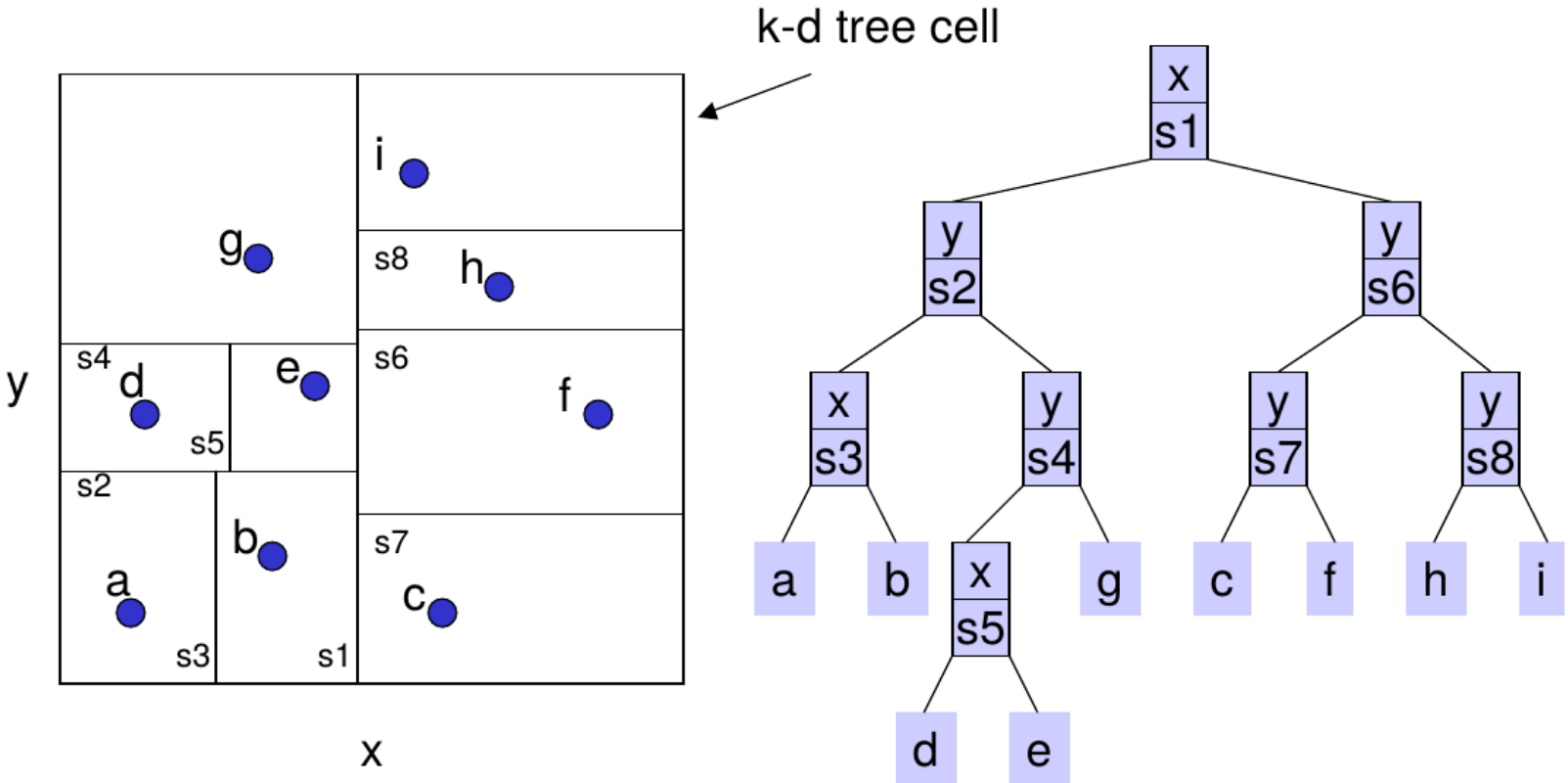




Finally


k-d tree cell
i
g
s8
h
s4
d
e
s6
f
y
s5
s2
b
s7
a
c
s3
s1
x
x
s1
y
s2
y
s6
x
s3
y
s4
y
s7
y
s8
a
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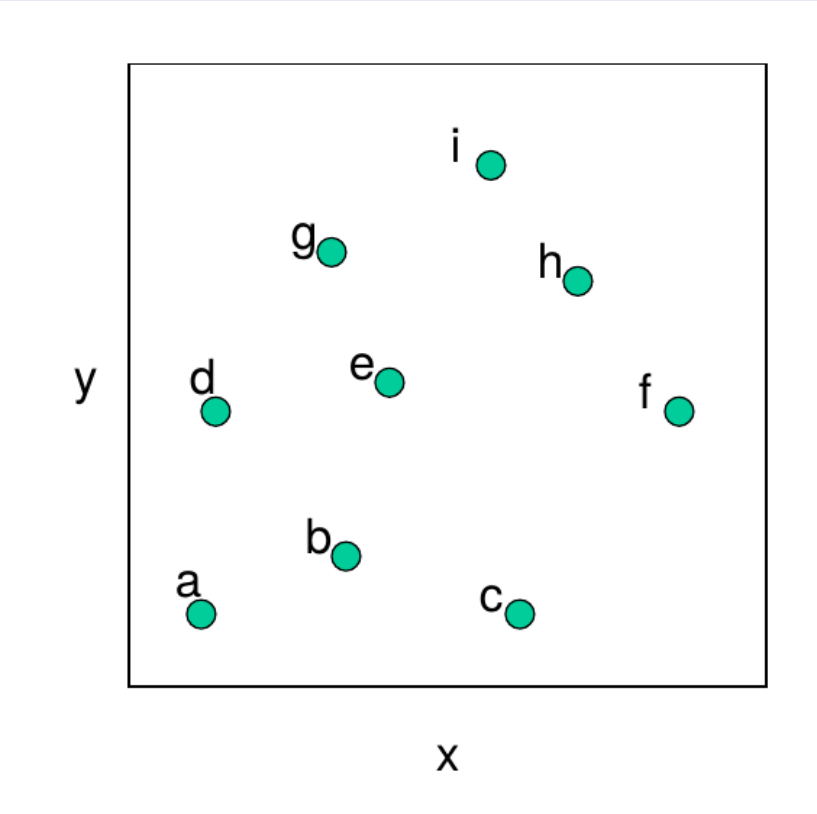
x
s5
g
c
f
h
i
d
e

Outline

We have the following

In each dimension we have certain sorting

	1	2	3	4	5	6	7	8	9
x	a	d	g	b	e	i	c	h	f
y	a	c	b	d	f	e	h	g	i



Therefore

The max spread is the argument that maximize the following quantities

$$\arg\max f_x - a_x$$
$$\arg\max g_y - a_y$$

Basically

- In the selected dimension the middle point in the list splits the data.

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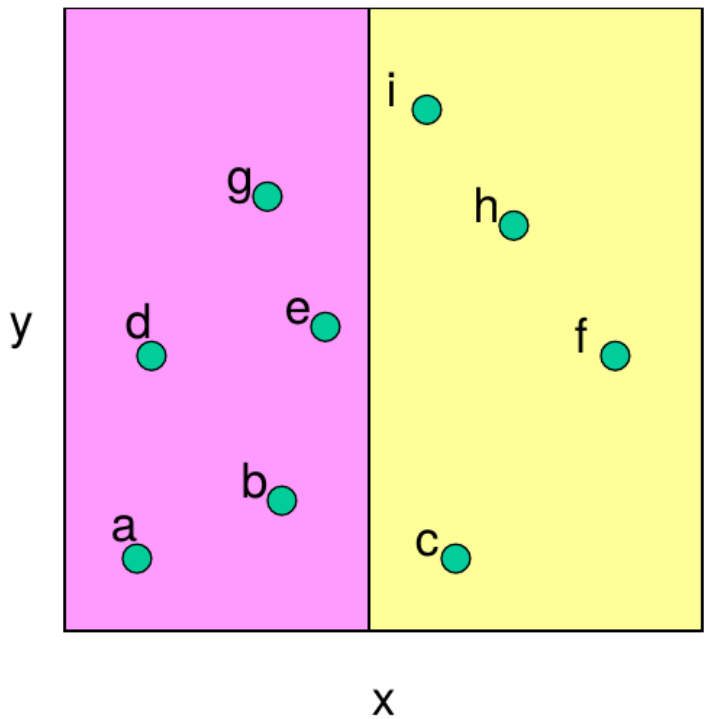

sorted points in each dimension

	1	2	3	4	5	6	7	8	9
x	a	d	g	b	e	i	c	h	f
y	a	c	b	d	f	e	h	g	i

indicator for each set

a	b	c	d	e	f	g	h	i
0	0	1	0	0	1	0	1	1

scan sorted points in y dimension and add to correct set

y	a	b	d	e	g	c	f	h	i

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KD Tree Construction Complexity

First sort the points in each dimension

- $O(dn \log n)$ time and dn storage.
- These are stored in matrices $A[1..d, 1..n]$

Finding the widest spread and equally divide

Into two subsets can be done in O(dn) time.

We have the recurrence

$$T(n, d) = 2T\left(\frac{n}{2}, d\right) + O(dn)$$

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Constructing the KD Tree can be done in

- Time $O(n \log n)$
- Space $O(n)$

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Node Structure

A node has 5 fields

- Axis (splitting axis)
- Value (splitting value)
- left (left subtree)
- right (right subtree)
- point (holds a point if left and right children are null)

Outline

Complexity

Theorem

A set of n points in the plane can be preprocessed in $O(dn \log n)$ time into a data structure of $O(dn)$ size so that any d-range query can be answered in time $O(d\sqrt{n} + k)$, where k is the number of answers reported

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Encoding Sets as Bit Vectors

Something Notable

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  - Size of intersection $= 3$; size of union $= 4$, Jaccard similarity (not distance) $= 3/4$
  - $d(C_1, C_2) = 1$–(Jaccard similarity) $= 1/4$

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  - 1 in row e and column s if and only if e is a member of s
  - Column similarity is the Jaccard similarity of the corresponding sets (rows with value 1)
  - **Typical matrix is sparse!**

Each document is a column

- Example: $sim(C_1, C_2) =$?
  - Size of intersection $= 3$; size of union $= 6$, Jaccard similarity (not distance) $= 3/6$
  - $d(C_1, C_2) = 1$–(Jaccard similarity) $= 3/6$

From Sets to Boolean Matrices

Rows

- Rows are equal to elements (shingles)

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Outline

Outline: Finding Similar Columns

So far and next goal

- So far:
  - Documents → Sets of shingles
  - Represent sets as boolean vectors in a matrix
- Next Goal: Find similar columns, Small signatures

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3. Optional: Check that columns with similar signatures are really similar

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Warnings

Comparing all pairs may take too much time: Job for Locality Sensitive Hashing (LSH)

- These methods can produce false negatives, and even false positives (if the optional check is not made)

Hashing Columns (Signatures)

Key idea

- "Hash" each column C to a small signature $h(C)$, such that:
  - (1) $h(C)$ is small enough that the signature fits in RAM.
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Finally, The Buckets

Buckets

- Thus, we hash documents into buckets, and expect that "most" pairs of near duplicate docs hash into the same bucket!

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Min-Hashing

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Imagine the rows of the boolean matrix permuted under random permutation π .

"Hash" function $h_\pi(C)$

- Define a "hash" function $h_\pi(C) =$ the number of the first (in the permuted order π) row in which column C has value 1:

$$h_\pi(C) = min_\pi \pi(C)$$

What can we do?

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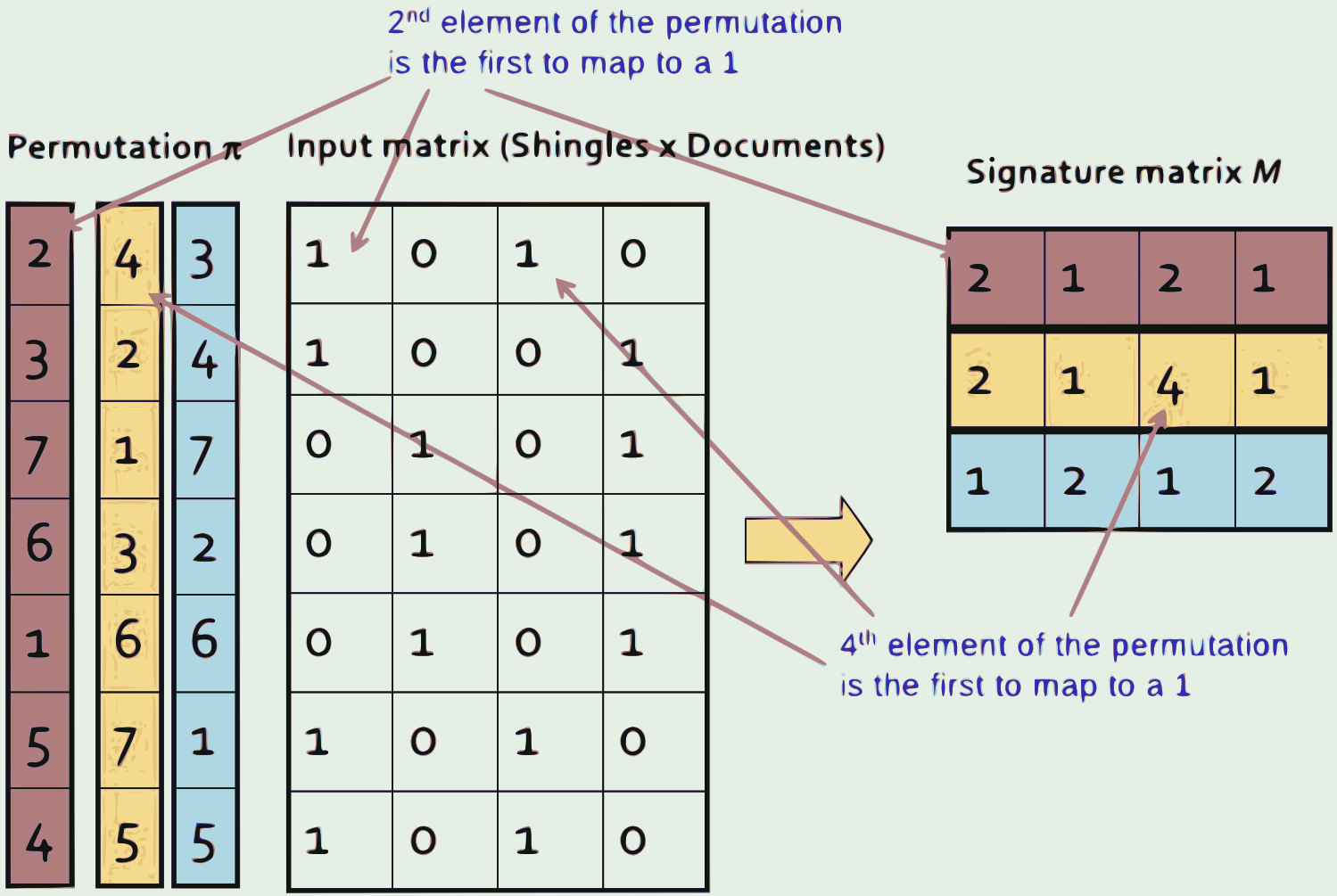
Min-Hashing Example

Something Notable



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Given cols C_1 and C_2, rows may be classified as

	C_1	C_2
A	1	1
B	1	0
C	0	1
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$a = \#$rows of type A, etc.

Note

$$sim(C_1, C_2) = \frac{a}{a+b+c} \tag{2}$$

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Note

- Because of the minhash property, the similarity of columns is the same as the expected similarity of their signatures

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- Because of the minhash property, the similarity of columns is the same as the expected similarity of their signatures

Similarity for Signatures

We know

- $Pr[h_\pi(C_1) = h_\pi(C_2)] = sim(C_1, C_2)$
- Now generalize to multiple hash functions

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Min-Hashing Example

Example

Permutation π | Input matrix (Shingles x Documents)

Permutation π			Input matrix (Shingles x Documents)			
2	4	3	1	0	1	0
3	2	4	1	0	0	1
7	1	7	0	1	0	1
6	3	2	0	1	0	1
1	6	6	0	1	0	1
5	7	1	1	0	1	0
4	5	5	1	0	1	0

Signature matrix M

2	1	2	1
2	1	4	1
1	2	1	2

Similarities:

	1-3	2-4	1-2	3-4
Col/Col	0.75	0.75	0	0
Sig/Sig	0.67	1.00	0	0

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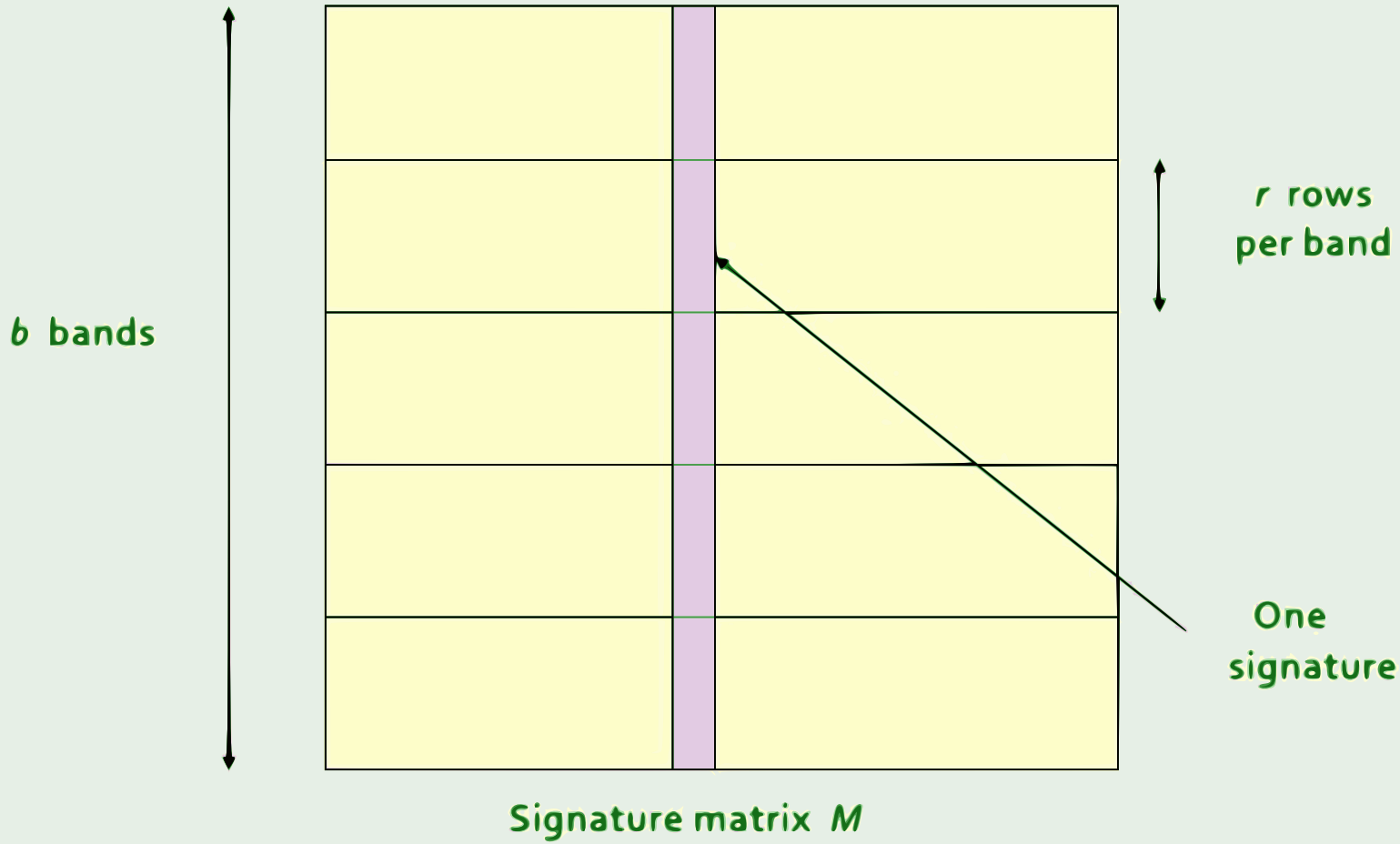

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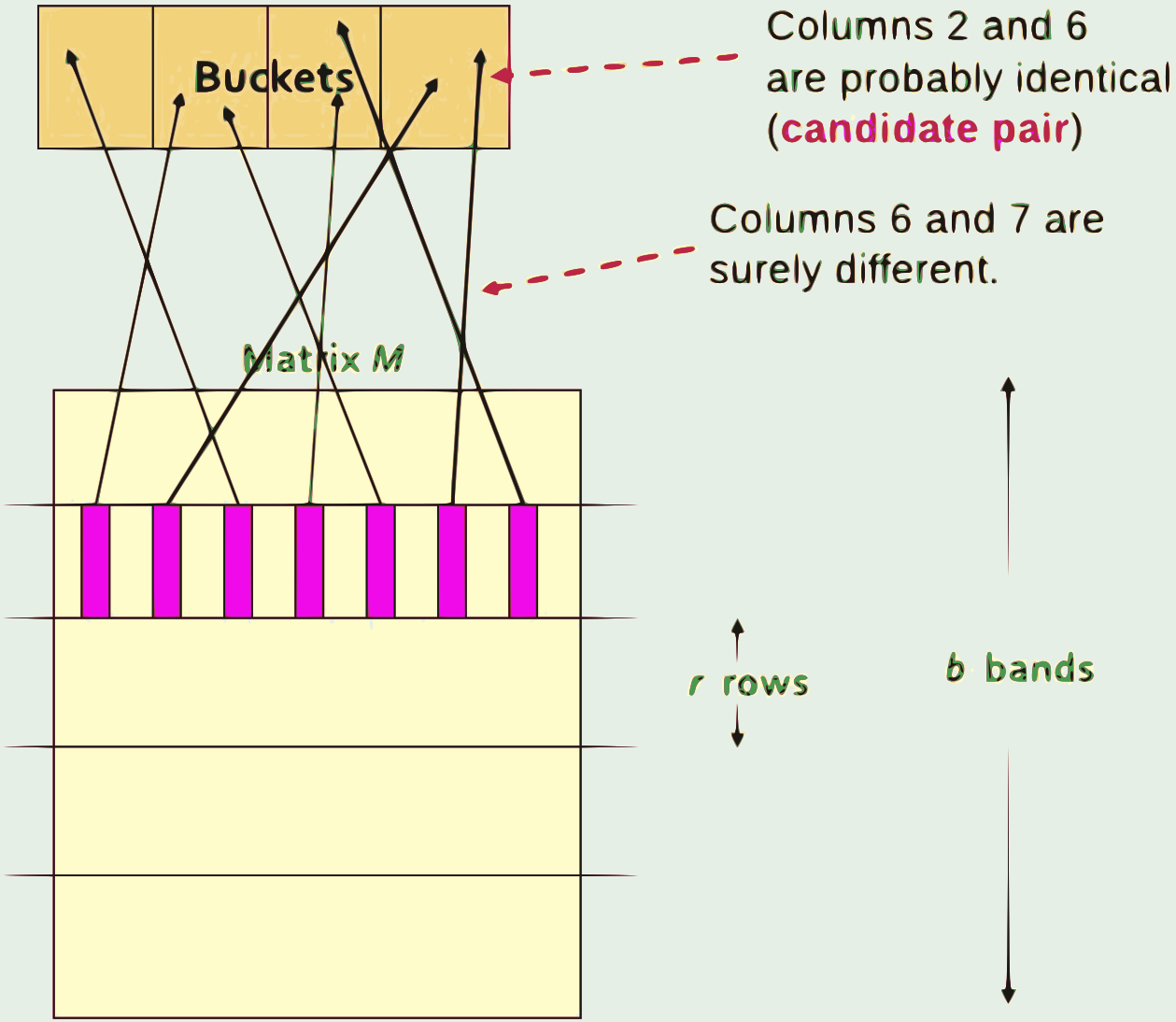

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Assume the following case

- Suppose $100,000$ columns of M ($100k$ docs)
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You need to pick

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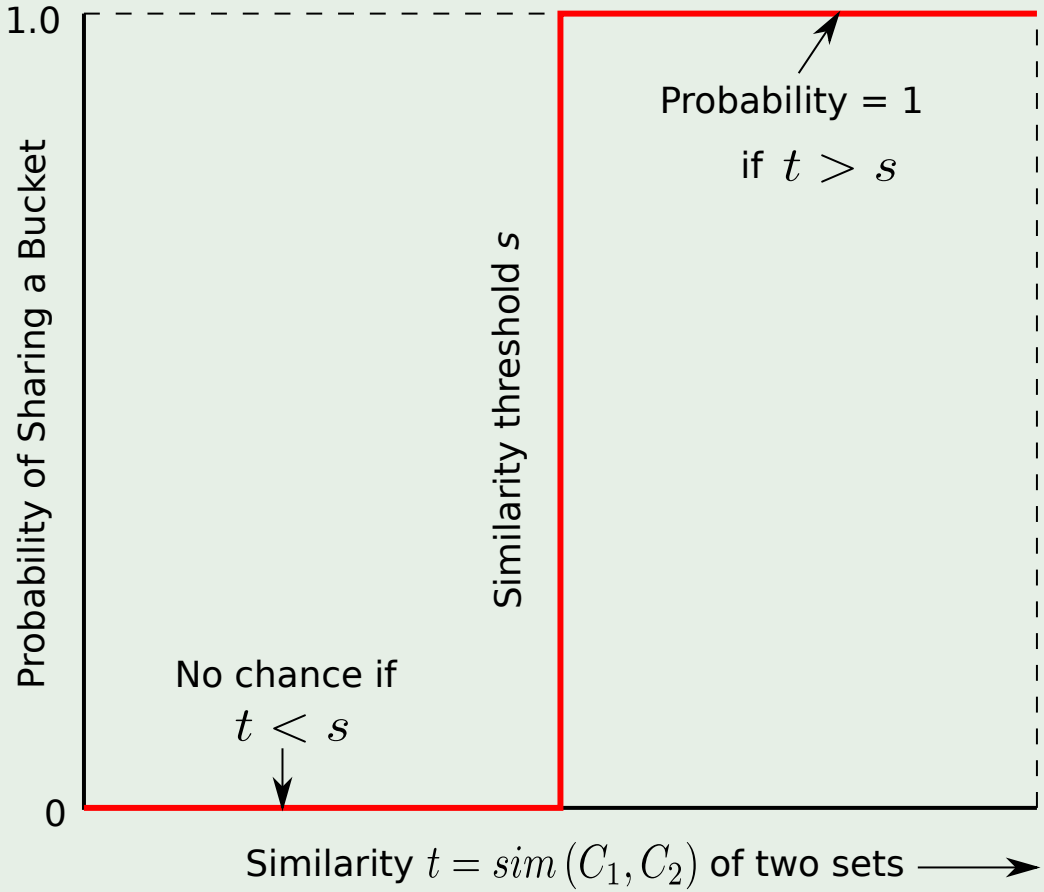
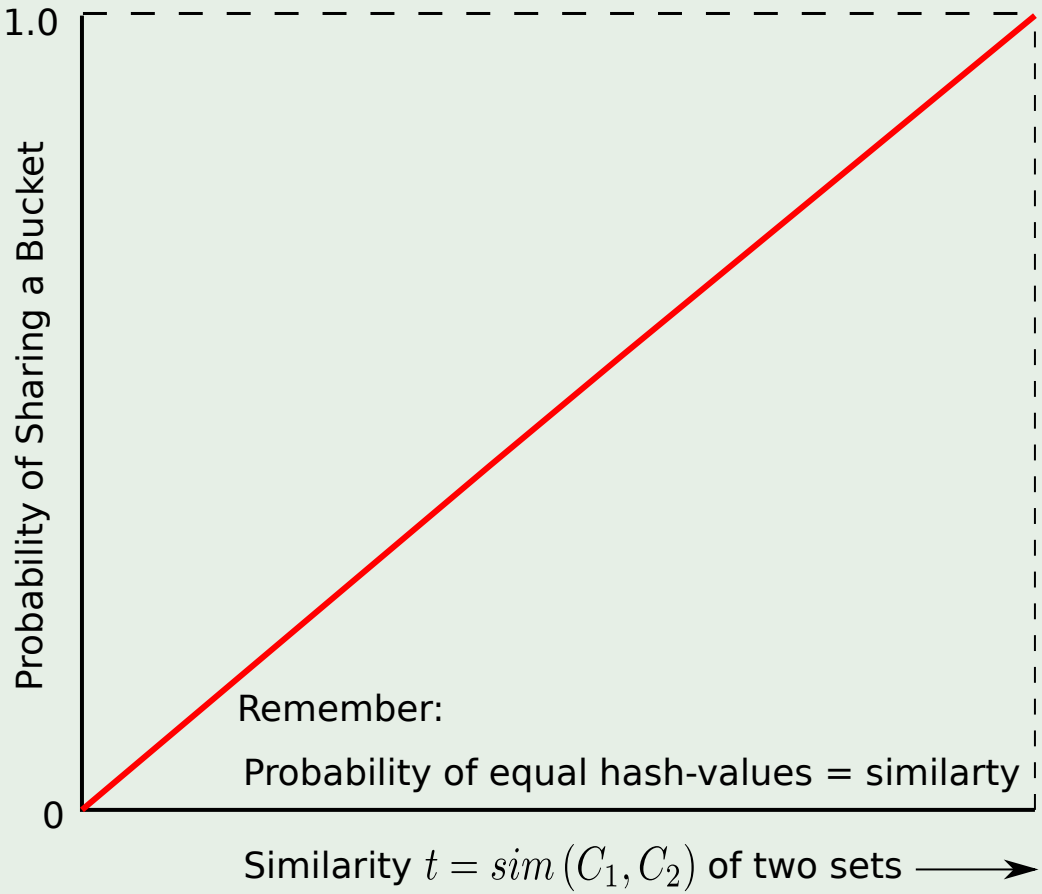
Analysis of LSH - What We Want

The Ideal detection of similar objects



What 1 Band of 1 Row Gives You

Not so great



Given that probability of two documents aggree in a row is s

We can calculate the probability that these documents become a candidate pair as follows

1. The probability that the signatures agree in all rows of one particular band is s^r.
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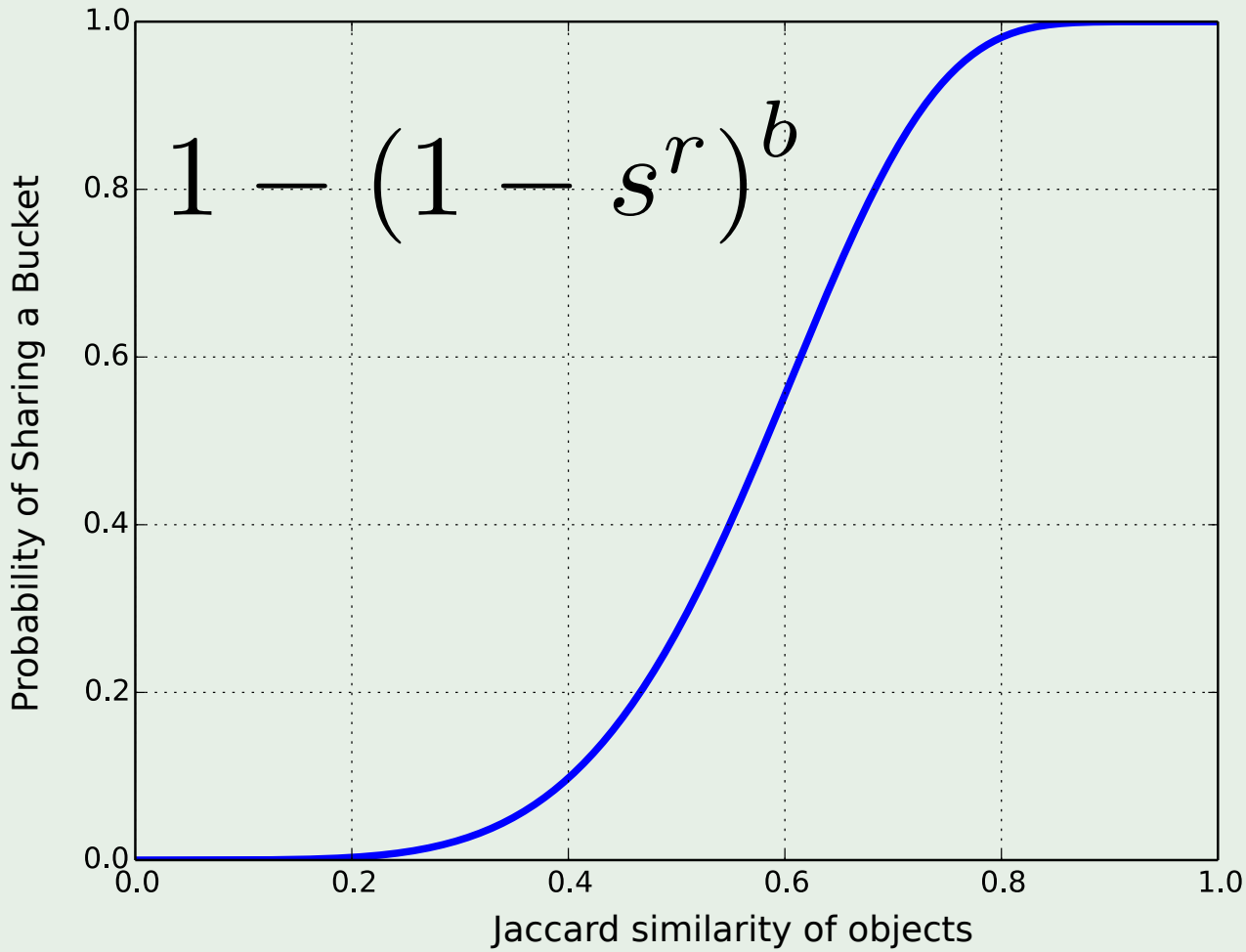
If you fix r and b

Something Notable



Example: $b = 20$; $r = 5$

Given

- Similarity threshold s

Similarity threshold s Prob. that at least 1 band is identical

s	$1 - (1 - s^r)^b$
.2	0.006
.3	0.047
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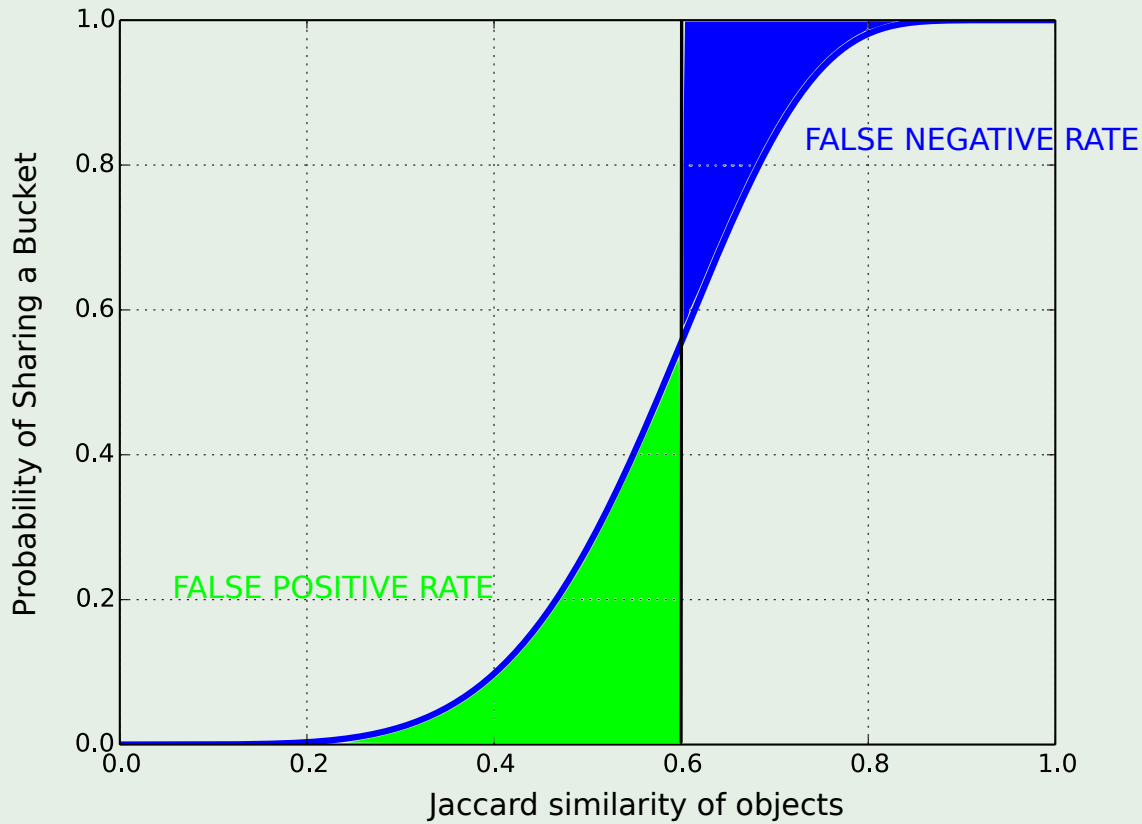
Picking r and b: The S-curve

Picking r and b to get the best S-curve

- 50 hash-functions $(r = 5, b = 10)$



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Tune M, b, r

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